Indian J. Phys. **52A**, 515–520 (1978)

Surface states of one dimensional deformed semi-infinite crystals

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(*Received* 9 *May* 1977, *revised* 7 *October* 1977)

Surface states are investigated for a one dimensional semi-infinite crystal deformed at the end Equation giving the surface state energy and the relevant existence condition are derived Making use of a numerical analysis, it is shown that the role of the existence condition becomes significant only for weak atomic potentials

1 Introduction

The theoretical investigation of surface states of various one dimensional semi-infinite systems, is a subject of considerable importance The earliest work in this direction is that of Tamm (1932) who studied a system which is very much idealised; the existence condition for Tamm's model was critically examined later by other authors (Roy & Tripathy 1977, Steslicka 1973). During the last two decades or so, several workers (Davison & Levine 1970, Steslicka 1973, Pharaseau 1960) have investigated one dimensional semi-infinite models, by taking account of distortions at the surface; such models are more realistic than the one treated by Tamm

In the present paper, we study the surface states for a semi-infinite one dimensional model deformed at the surface. We have derived the equation determining the energy of surface states and the relevant existence condition The role of existence condition in relation to surface states, has been found to be highly important (Roy & Tripathy 1977) In view of this, we have presented a detailed quantitative analysis of the existence condition for the model under consideration and examined the circumstances under which this condition is likely to play a significant part

2 Model and Derivation of Formulae

The model trated is shown in Fig 1 The deformation is characterised by the displacement Δ of the surface atom with respect to its periodic position i.e. $x = 0$ This kind of deformation is akin to experimental findings (Philips 1974) In our model, the atomic potentials are represented by δ-functions of

strength P, this strength is, as is well known, realisable as a limiting value of rectangular barrier potential;

$$P = \operatorname{Lim} \frac{mV_1}{\hbar^2} b_1 a$$

$$b_1 \to 0$$
$$V_1 \to \infty$$

In the above form of P, V_1 and b_1 are respectively the height and width of the barrier. The mass m of the electron and $\hbar^2$ ($\hbar = h/2\pi$) as well as a, are introduced for the purpose of securing compactness in the final form of some equations (e.g. the Kronig-Penney equation (8)).

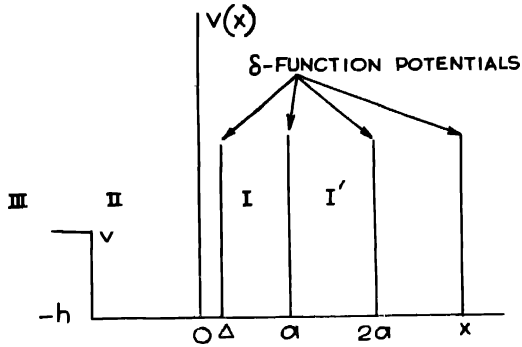

Fig 1. Model of a one dimensional semi-infinite crystal with distortion at the surface. $V(x)$ is the P.E. of the electron. The atomic potentials are characterised by δ-functions of strength 'P', as explained in the text. The distortion is described by the displaced position of the surface atom.

Now, to derive the equations determining the energies of the surface states, we note first that the wave functions for various regions along x-axis, have the following forms

$$\psi_{I'} = D(e^{i\alpha x} + \lambda e^{-i\alpha x}), \qquad \text{for region I',} \qquad \ldots (1)$$

$$\psi_1 = A_0 e^{i\alpha x} + B_0 e^{-i\alpha x}, \qquad \text{for region I,}$$

$$\psi_2 = Ae^{i\alpha x} + Be^{-i\alpha x}, \qquad \text{for region II,} \qquad (3)$$

$$\psi_3 = Ce^{\gamma x}, \qquad \text{for region III,} \qquad (4)$$

The symbols have meanings as given below:

$$\alpha^2 = \frac{2mE}{\hbar^2}, \quad \gamma^2 = \frac{2m}{\hbar^2}(V-E), \qquad \lambda = \frac{e^{-i\mu a}}{e^{i\mu a}}$$

μ is the wave vector and E is the energy of the electron while D, A_0 ... etc. are arbitrary constants.

Subjecting the above wave functions to the requisite boundary conditions (i.e. the continuity of the wave functions and their derivatives) at $x = -b$, Δ and a, we get a system of six homogeneous algebraic equations in terms of the constants D, A_0, B_0, A, B and C. In order that these equations have non-trivial solutions for the six constants, the determinant of the (6×6) matrix formed by the co-efficients of D, A_0, ... etc., must be zero. This condition leads us to the following equation :

$$e^{i\mu a} = \cos\chi + \frac{\sin\chi}{\chi} f \qquad \ldots (5)$$

where,

$$f = \frac{g\left(1+\frac{2P\Delta}{a}\right)(\chi + 2P\sin\chi\cos\chi) - 2P\cos^2\chi\left(1-\frac{2P\Delta}{a}\right)}{\left(1-\frac{2P\Delta}{a}\right)\left\{1-\frac{2P}{\chi}\sin\chi\cos\chi\right\} - \frac{2P}{\chi}g\left(1+\frac{2P\Delta}{a}\right)\sin^2\chi} \qquad (6)$$

$$g = \frac{(\phi^2-\chi^2)^{\frac{1}{2}}\cos(t\chi) - \chi\sin(t\chi)}{(\phi^2-\chi^2)^{\frac{1}{2}}\sin(t\chi) + \chi\cos(t\chi)} \qquad \ldots (7)$$

The entities χ and μ also satisfy the well known Kronig-Penney equation.

$$\cos\mu a = \cos\chi + \frac{P\sin\chi}{\chi} \qquad \ldots (8)$$

The wave vector μ corresponding to the surface states occurring in the n-th forbidden gap, is characterised by the following complex form (Tamm 1932).

$$\mu = ik + \frac{n\pi}{a} \qquad \ldots (9)$$

where k is positive. Combining (5). (8) and (9), we get

$$2P\chi\cot\chi = \chi^2 + f^2 - 2Pf. \qquad \ldots (10)$$

We now want to establish the condition which would guarantee that k is positive-definite. To do so, we restore (9) in (5) and (8) and subtract one of the resulting equations from the other. This gives us the following equation :

$$(-1)^n \sin h(ka) = (P-f)\frac{\sin\chi}{\chi} \qquad \ldots (11)$$

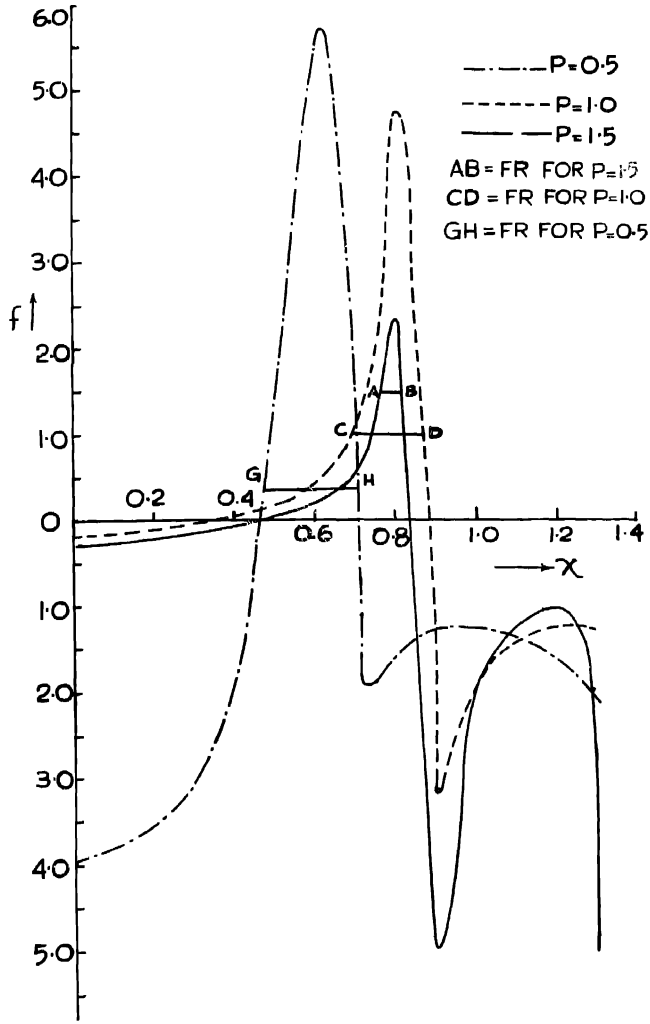

Fig. 2 Plot of f versus χ, both of which are dimensionless. *FR* denotes forbidden range of χ values in accordance with condition (12) in the text. For all curves, $\phi = 1{\cdot}3$, $\Delta/a = 0{\cdot}1$, $h/a = t = 1{\cdot}1$.

We note that, for positive k, $\sin h(ka)$ is always positive. Further, for the n-th gap, $n\pi < \chi < (n+1)\pi$ hence, $\frac{\sin \chi}{\chi}$ has same sign as $(-1)^n$. Thus for the compatibility of signs of both sides of (11) we must have

$$P \quad /$$

3 Numerical Analysis and Discussion

The condition (12) gives the so-called existence condition for the surface states of model of Fig. 1. The energies characteristic of surface states correspond to such values of χ as simultaneously satisfy the eq. (11) and the existence condition (12). We wish to report in future, numerical estimates of surface-states in the light of similar results obtained by others (Neuberger & Fischer 1975). In this paper, we only present a numerical analysis of the existence condition (12). As mentioned in the introduction, the study of such conditions occupies by itself an important place in the arena of surface-states (Roy & Tripathy 1977). For different values of P and fixed values of ϕ, t and (Δ/a), the graphs in figures 2 and 3, show the variations of f with χ. The regions of χ [illegible] $f > 1$, give

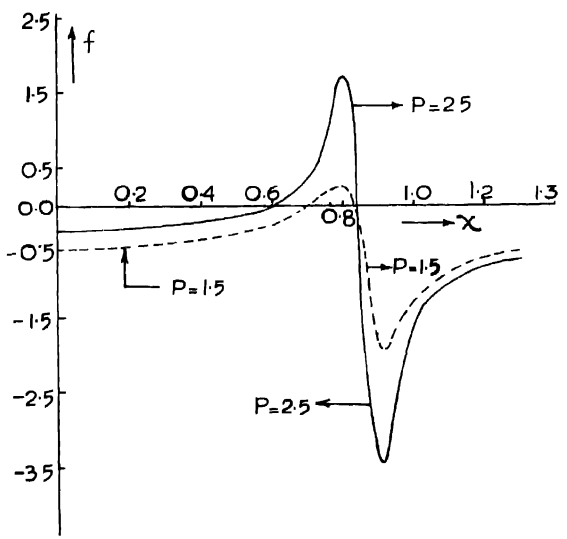

Fig. 3. Same kind of graphs as in Fig. 2, for $P = 2.5$ and 3.5. The parameters ϕ, Δ/a and t are the same as before. There are no forbidden regions for these conditions.

the values of χ for which no surface-states can occur; the energies which the existence condition (12) prohibits, are proportional to the squares of values of χ just mentioned.

From the graphs, it is seen that for $P = 0{\cdot}5$, $1{\cdot}0$ and $1{\cdot}5$, there appear a forbidden region of energy. But, for $P = 2{\cdot}5$ and $3{\cdot}5$, the existence condition, on its own, permits all energies from zero upto the highest permissible value, ϕ ($= 1{\cdot}3$, for our case). Further, with decrease of P, the width of the forbidden range becomes larger and the lower edge of the forbidden range assumes smaller value of energy. Thus, we can conclude that the role of existence condition is generally significant for small values of P i.e., for weak atomic potentials.

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